

Researchers determine naphthalene concentrations in the air

October 4 2016



Credit: National Research Nuclear University

Researchers from the National Research Nuclear University MEPhI (Russia) have investigated possible structures of the naphthalene dimer in different states in order to better understand the photochemical properties of naphthalene and to estimate its concentrations in the air based on spectral measurements.

Naphthalene is a toxic hydrocarbon. The International Agency for Research on Cancer (IARC) classifies naphthalene as possibly carcinogenic to humans and animals.

Researchers analyzed the possible structures of naphthalene dimers, a

combination of two naphthalene molecules. These naphthalene molecules were studied in the ground and excited (excimer) [electronic states](#) using DFT-D and TDDFT-D methods, which are used to analyze the nature of electronic states and calculate their electronic transition energies.

The presence and concentration of naphthalene and naphthalene dimers in the air are estimated on the basis of information about the position of spectral absorption bands. MEPhI researchers have learned to obtain this information using a novel method of [quantum chemical calculations](#).

The presence of naphthalene dimer in the air indicates a quite high naphthalene concentration, said Alexander Bagaturyants, Professor at the Department of Condensed Matter Physics at MEPhI, Photochemistry Center of the Russian Academy of Sciences.

"We have calculated the corresponding binding and electronic transition energies, analyzed the nature of the electronic states in different structures, and found several parallel (stacked) and T-shaped structures in both the ground and excited (excimer) states in a rather narrow energy range," Alexander Bagaturyants said.

According to the scientist, their research has contributed to the excimer theory—an excimer is a combination of two identical molecules in an excited state—including the study of naphthalene excimers.

The results of this research have been published in the *Journal of Physical Chemistry* of the American Chemical Society (ACS).

Provided by National Research Nuclear University

Citation: Researchers determine naphthalene concentrations in the air (2016, October 4)

retrieved 11 May 2024 from <https://phys.org/news/2016-10-naphthalene-air.html>

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